10/735,499

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	184	514/490 or 560/133	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	ON	2006/12/28 04:52
L2	13	l1 and (integrin or phenylalanine)	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	ON	2006/12/28 04:59
L3	1	("6689781").PN.	USPAT	OR	OFF	2006/12/28 07:28
L4	1	("6291453").PN.	USPAT	OR	OFF	2006/12/28 07:29
L5	1	("6492421").PN.	USPAT	OR	OFF	2006/12/28 08:08
L6	1	("6689781").PN.	USPAT	OR	OFF	2006/12/28 08:08

10/735,499

STN SEARCH TRANSCRIPT

```
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 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  AUG 09   INSPEC enhanced with 1898-1968 archive
 NEWS  4  AUG 28   ADISCTI Reloaded and Enhanced
 NEWS  5  AUG 30   CA(SM)/CAplus(SM) Austrian patent law changes
 NEWS  6  SEP 21   CA/CAplus fields enhanced with simultaneous left and right
                   truncation
 NEWS  7  SEP 25   CA(SM)/CAplus(SM) display of CA Lexicon enhanced
 NEWS  8  SEP 25   CAS REGISTRY(SM) no longer includes Concord 3D coordinates
 NEWS  9  SEP 25   CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
 NEWS 10  SEP 28   CEABA-VTB classification code fields reloaded with new
                   classification scheme
 NEWS 11  OCT 19   LOGOFF HOLD duration extended to 120 minutes
 NEWS 12  OCT 19   E-mail format enhanced
 NEWS 13  OCT 23   Option to turn off MARPAT highlighting enhancements available
 NEWS 14  OCT 23   CAS Registry Number crossover limit increased to 300,000 in
                   multiple databases
 NEWS 15  OCT 23   The Derwent World Patents Index suite of databases on STN
                   has been enhanced and reloaded
 NEWS 16  OCT 30   CHEMLIST enhanced with new search and display field
 NEWS 17  NOV 03   JAPIO enhanced with IPC 8 features and functionality
 NEWS 18  NOV 10   CA/CAplus F-Term thesaurus enhanced
 NEWS 19  NOV 10   STN Express with Discover! free maintenance release Version
                   8.01c now available
 NEWS 20  NOV 20   CAS Registry Number crossover limit increased to 300,000 in
                   additional databases
 NEWS 21  NOV 20   CA/CAplus to MARPAT accession number crossover limit increased
                   to 50,000
 NEWS 22  DEC 01   CAS REGISTRY updated with new ambiguity codes
 NEWS 23  DEC 11   CAS REGISTRY chemical nomenclature enhanced
 NEWS 24  DEC 14   WPIDS/WPINDEX/WPIX manual codes updated
 NEWS 25  DEC 14   GBFULL and FRFULL enhanced with IPC 8 features and
                   functionality
 NEWS 26  DEC 18   CA/CAplus pre-1967 chemical substance index entries enhanced
                   with preparation role
 NEWS 27  DEC 18   CA/CAplus patent kind codes updated
 NEWS 28  DEC 18   MARPAT to CA/CAplus accession number crossover limit increased
                   to 50,000
 NEWS 29  DEC 18   MEDLINE updated in preparation for 2007 reload
 NEWS 30  DEC 27   CA/CAplus enhanced with more pre-1907 records

 NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8
 NEWS X25      X.25 communication option no longer available

 NEWS PRICE    STN 2007 Prices

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 07:51:15 ON 28 DEC 2006

=> file registry
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY     SESSION
FULL ESTIMATED COST                                       0.21        0.21

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DICTIONARY FILE UPDATES:  27 DEC 2006  HIGHEST RN 916420-05-8

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http://www.cas.org/ONLINE/UG/regprops.html

=>
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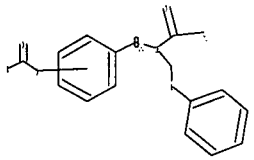
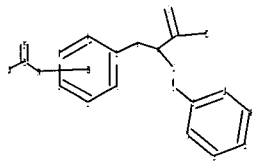




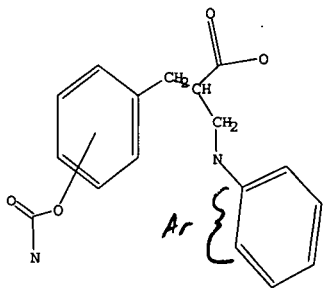
chain nodes :
7 8 9 10 11 19 20 24 25 26
ring nodes :
1 2 3 4 5 6 12 13 14 15 16 17
ring/chain nodes :
27
chain bonds :
5-7 7-8 8-9 8-10 9-19 9-20 10-11 11-12 24-25 25-26 25-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
exact/norm bonds :
9-19 9-20 10-11 11-12 24-25 25-26 25-27
exact bonds :
5-7 7-8 8-9 8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:Atom

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



ONLY Ar = HETEROARYL COMPOUNDS WERE EXEMPLIFIED IN THE APPLICATION, THIS IS WHY NO HITS IN THE PRIOR ART - OR AT LEAST THE REASON WHY APPLICANTS' OWN WORK DID NOT COME UP.

Structure attributes must be viewed using STN Express query preparation.

=> S L1
SAMPLE SEARCH INITIATED 07:51:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 833 TO 1807
PROJECTED ANSWERS: 0 TO 0

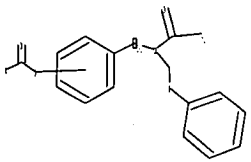
L2 0 SEA SSS SAM L1

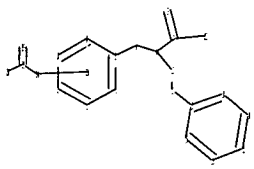
=> S L1 SSS FULL
FULL SEARCH INITIATED 07:51:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1250 TO ITERATE

100.0% PROCESSED 1250 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>
=>
Uploading C:\Program Files\Stnexp\Queries\PHENYLALANINE INTEGRIN INHs.str





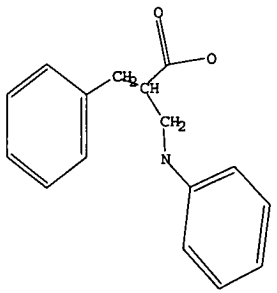
chain nodes :
7 8 9 10 11 19 20 24 25 26
ring nodes :
1 2 3 4 5 6 12 13 14 15 16 17
ring/chain nodes :
27
chain bonds :
5-7 7-8 8-9 8-10 9-19 9-20 10-11 11-12 24-25 25-26 25-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
exact/norm bonds :
9-19 9-20 10-11 11-12 24-25 25-26 25-27
exact bonds :
5-7 7-8 8-9 8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:Atom

L4 STRUCTURE UPLOADED

=> D L4
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L4
SAMPLE SEARCH INITIATED 08:10:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 486 TO ITERATE

100.0% PROCESSED 486 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8398 TO 11042
PROJECTED ANSWERS: 2 TO 124

L5 2 SEA SSS SAM L4

=> S L4 SSS FULL
FULL SEARCH INITIATED 08:10:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9865 TO ITERATE

100.0% PROCESSED 9865 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L6 7 SEA SSS FUL L4

=> FILE CAPLUS
COST IN U.S. DOLLARS SINCE FILE ENTRY 347.08 TOTAL SESSION 347.29

FULL ESTIMATED COST

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=> S L6
L7 4 L6

=> D 1-4 IBIB ABS HITSTR

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:869580 CAPLUS
DOCUMENT NUMBER: 137:353320
TITLE: Preparation of amino(oxo)acetic acid derivatives as selective protein tyrosine phosphatase inhibitors
INVENTOR(S): Liu, Gang; Xin, Zhili; Pei, Zhonghua; Li, Xiaofeng; Szczepankiewicz, Bruce G.; Janowick, David A.; Oost, Thorsten K.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 60 pp., Cont.-in-part of U.S. Pat. Appl. 2002 72,516.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002169157	A1	20021114	US 2002-85157	20020227
US 2002035137	A1	20020321	US 2001-918928	20010731
US 2002072516	A1	20020613	US 2001-941471	20010829
US 6972340	B2	20051206		
WO 2003072537	A2	20030904	WO 2003-US3663	20030206
WO 2003072537	A3	20031218		

W: CA, JP, MX
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR

PRIORITY APPLN. INFO.:		
US 2000-228651P	P	20000829
US 2000-650922	A2	20000829
US 2001-918928	A2	20010731
US 2001-941471	A2	20010829
US 2002-85157	A	20020227

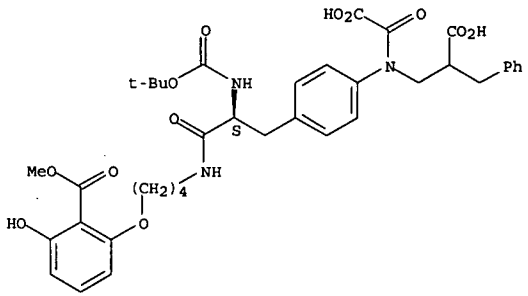
OTHER SOURCE(S): MARPAT 137:353320

AB Compds. B-L-A-N(D)COCO2P2 [A are rings of defined structure; B = H, alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; D = substituted Ph, alkyl, or 1-alkenyl [the substituent at the o- or 2-position is alkoxy, alkyl, sulfamoyl, amino, cyano, nitro, CO2P1, SO3H, P(O)(OH)2, CH2P(O)(OH)2, CHFP(O)(OH)2, CF2P(O)(OH)2, or C(:NH)NH2] or certain 5-membered heterocycles; P1, P2 = H, alkyl, alkenyl, arylalkyl, cycloalkyl, cycloalkylalkyl; L = (un)substituted (hetero)alkylene] or their therapeutically acceptable salts were prepared as protein tyrosine kinase 1B (PTP1B) inhibitors. Thus, N-[5-[[N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl]amino]pentanoyl]-L-methionine and Me 2-[4-[[N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl]amino]-3-ethylphenylalanyl)amino]butoxy]-6-hydroxybenzoate were prepared and showed Kic = 0.077 ± 0.012 and 0.016 ± 0.003 μM, resp., for inhibition of PTP1B.

IT 474917-46-9P 474917-51-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino(oxo)acetic acid derivs. as selective protein tyrosine phosphatase inhibitors)

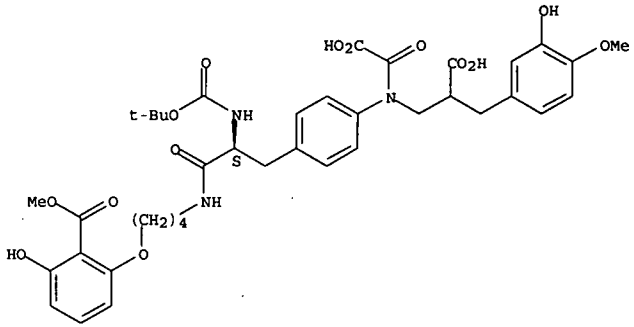
RN 474917-46-9 CAPLUS
CN Benzenepropanoic acid, α-[[(carboxycarbonyl)[4-[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[4-[3-hydroxy-2-(methoxycarbonyl)phenoxy]butyl]amino]-3-oxopropyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 474917-51-6 CAPLUS
CN Benzenepropanoic acid, α-[[(carboxycarbonyl)[4-[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[4-[3-hydroxy-2-(methoxycarbonyl)phenoxy]butyl]amino]-3-oxopropyl]phenyl]amino]methyl]-3-hydroxy-4-methoxy- (9CI) (CA INDEX NAME)

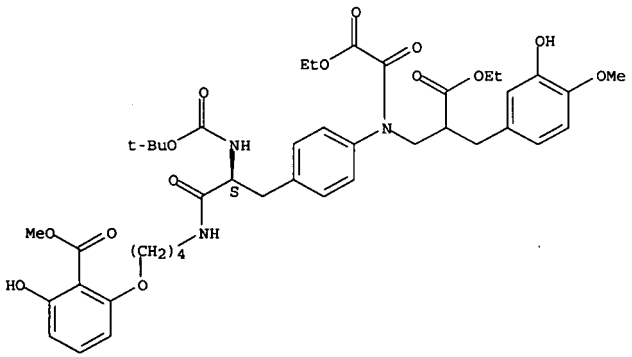
Absolute stereochemistry.



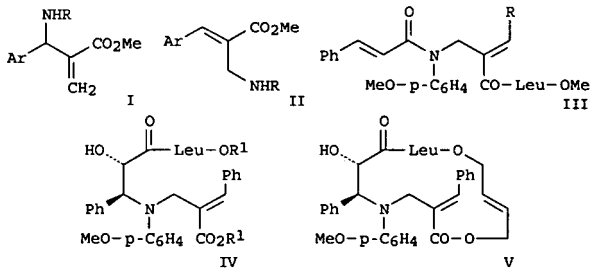
IT 474917-89-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino(oxo)acetic acid derivs. as selective protein tyrosine

phosphatase inhibitors)
RN 474917-89-0 CAPLUS
CN Benzenepropanoic acid, α-[[[4-[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[4-[3-hydroxy-2-(methoxycarbonyl)phenoxy]butyl]amino]-3-oxopropyl]phenyl](ethoxyoxoacetyl)amino]methyl]-3-hydroxy-4-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

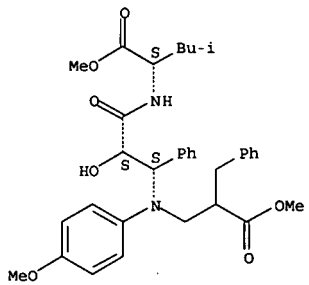


L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:746515 CAPLUS
DOCUMENT NUMBER: 137:385103
TITLE: Palladium(0)-Catalyzed Regioselective Synthesis of α-Dehydro-β-amino Esters from Amines and Allyl Acetates: Synthesis of a α-Dehydro-β-amino Acid Derived Cyclic Peptide as a Constrained β-Turn Mimic
AUTHOR(S): Rajesh, S.; Banerji, Biswadip; Iqbal, Javed
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Kanpur, 208 016, India
SOURCE: Journal of Organic Chemistry (2002), 67(22), 7852-7857
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:385103
GI



AB Baylis-Hillman allyl acetates ArCH(OAc)C(:CH2)CO2Me (Ar = Ph, C6H4OMe-4, C6H4Cl-4) react regioselectively with primary amines H2NR (R = Ph, C6H4OMe-4, C6H4Me-4, C6H4Cl-4) in the presence of palladium(0) catalyst to afford α-dehydro-β-amino esters I and II. The regioselectivity of the reaction can be controlled by temperature and reaction medium leading to the synthesis of regioisomers I and II. II is a turn inducer, and the dipeptides III (R = Ph, Bu-i) derived from it show the presence of an eight-membered intramol. hydrogen bond. Also, CoCl2 catalyzes the cleavage of N-(2,3-epoxycinnamoyl)-L-leucine Me ester with α-dehydro-β-amino acid derivative II (Ar = Ph, R = C6H4OMe-4) to afford the corresponding dipeptide derivs. IV (R1 = Me), which exhibit an intramol. hydrogen bond and thus mimic a β-turn. This intramol. hydrogen bonding preorganizes the corresponding diallylated peptide IV (R1 = CH2CH:CH2) for cyclization via ring-closing metathesis to afford the cyclic peptide V as a constrained mimic of a β-turn.
IT 450416-52-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of a dipeptide diallyl ester from its Me ester precursor)
RN 450416-52-1 CAPLUS
CN L-Leucine, (2S,3S)-2-hydroxy-N-[3-methoxy-3-oxo-2-(phenylmethyl)propyl]-N-(4-methoxyphenyl)-3-phenyl-β-alanyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



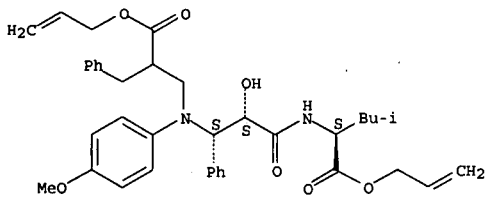
IT 450416-54-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(ring-closing metathesis of dipeptide diallyl esters with intramol. hydrogen bonding)

RN 450416-54-3 CAPLUS

CN L-Leucine, (2S,3S)-2-hydroxy-N-(4-methoxyphenyl)-N-[3-oxo-2-(phenylmethyl)-3-(2-propenyloxy)propyl]-3-phenyl-β-alanyl-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:37249 CAPLUS

DOCUMENT NUMBER: 137:185792

TITLE: Synthesis of an α-dehydro β-amino acid derived cyclic peptide as a constrained β-turn mimic

AUTHOR(S): Rajesh, S.; Srivastava, Jyoti; Bannerji, Biswadip; Iqbal, Javed

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Kanpur, 208 016, India

SOURCE: ARKIVOC [online computer file] (2001), 2(10), No pp. given
CODEN: AKVCFI
URL: http://www.arkat.org/arkat/journal/Govi/Govi2.pdf

PUBLISHER: ARKAT Foundation

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:185792

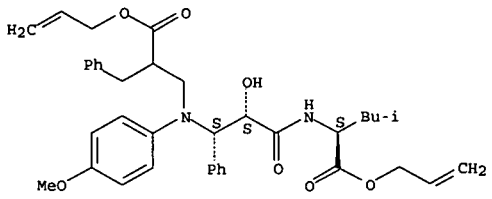
AB Cobalt(II) chloride catalyzes the cleavage of epoxy peptides with an α-dehydro β-amino acid derivative to afford the corresponding dipeptide derivative which exhibits an intramol. hydrogen bond and thus mimics a β-turn. This intramol. hydrogen bonding preorganizes the corresponding diallylated peptide for cyclization via ring closing metathesis to afford the cyclic peptide as a constrained mimic of a β-turn.

IT 450416-54-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dehydro beta amino acid derived cyclic peptide as constrained beta turn mimic with intramol. hydrogen bond)

RN 450416-54-3 CAPLUS

CN L-Leucine, (2S,3S)-2-hydroxy-N-(4-methoxyphenyl)-N-[3-oxo-2-(phenylmethyl)-3-(2-propenyloxy)propyl]-3-phenyl-β-alanyl-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

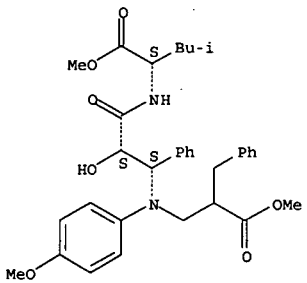


IT 450416-52-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dehydro beta amino acid derived cyclic peptide as constrained beta turn mimic with intramol. hydrogen bond)

RN 450416-52-1 CAPLUS

CN L-Leucine, (2S,3S)-2-hydroxy-N-[3-methoxy-3-oxo-2-(phenylmethyl)propyl]-N-(4-methoxyphenyl)-3-phenyl-β-alanyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:234566 CAPLUS

DOCUMENT NUMBER: 131:44796

TITLE: Solid-Phase Synthesis of 3,4,5-Substituted 1,5-Benzodiazepin-2-ones

AUTHOR(S): Lee, Jung; Gauthier, Diane; Rivero, Ralph A.

CORPORATE SOURCE: The R.W. Johnson Pharmaceutical Research Institute, Spring House, PA, 19477, USA

SOURCE: Journal of Organic Chemistry (1999), 64(9), 3060-3065
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

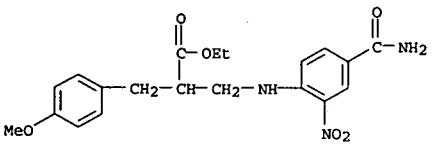
OTHER SOURCE(S): CASREACT 131:44796

AB The preparation of 3,4,5-substituted 8-carboxamido-1,5-benzodiazepin-2-ones using a solid-phase synthetic method is described. 4-Fluoro-3-nitrobenzoic acid is tethered to a solid support via the acid group. Aromatic substitution of the aryl fluoride with either an α- or

β-substituted β-amino ester is carried out in the presence of DIEA in DMF. The reduction of the aryl nitro group is accomplished in the presence of $SnCl_2 \cdot H_2O$. Hydrolysis of the ester is carried out in the presence of a heterogeneous mixture of 1 N NaOH/THF (1:1). The resulting aniline acid is cyclized to form the benzodiazepinone skeleton with DIC and HOBt. Selective alkylation at the N-5 position of the benzodiazepinone is accomplished with alkyl halides in the presence of K_2CO_3 in acetone. The desired products are cleaved from solid supports and obtained in 46-98% isolated yields.

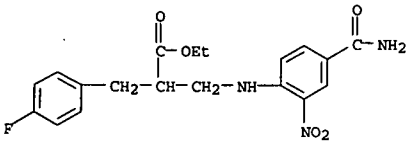
IT 224811-62-5P 224811-63-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of benzodiazepinones)

RN 224811-62-5 CAPLUS
CN Benzenepropanoic acid, α-[[[4-(aminocarbonyl)-2-nitrophenyl]amino]methyl]-4-methoxy-, ethyl ester (9CI) (CA INDEX NAME)



CITED AS CLOSEST PRIOR ART.

RN 224811-63-6 CAPLUS
CN Benzenepropanoic acid, α-[[[4-(aminocarbonyl)-2-nitrophenyl]amino]methyl]-4-fluoro-, ethyl ester (9CI) (CA INDEX NAME)



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NEWS	27	DEC 18	CA/CAplus patent kind codes updated
NEWS	28	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
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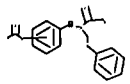
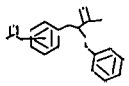
=>
Uploading C:\Program Files\Stnexp\Queries\PHENYLALANINE INTEGRIN INHs.str





chain nodes :

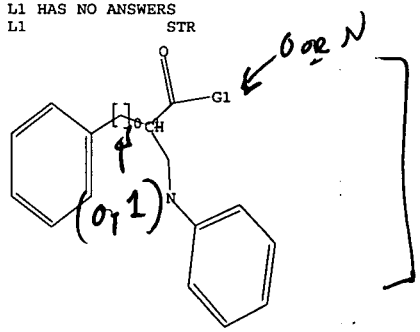
7 8 9 10 11 19 20 24 25 26
ring nodes :
1 2 3 4 5 6 12 13 14 15 16 17
ring/chain nodes :
27
chain bonds :
5-7 7-8 8-9 8-10 9-19 9-20 10-11 11-12 24-25 25-26 25-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
exact/norm bonds :
9-19 9-20 10-11 11-12 24-25 25-26 25-27
exact bonds :
5-7 7-8 8-9 8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:Atom

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



FULL SCOPE OF CL. 1, 2 SEARCH

G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> S L1
SAMPLE SEARCH INITIATED 09:00:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1074 TO ITERATE

100.0% PROCESSED 1074 ITERATIONS 50 ANSWERS
SEARCH TIME: 00.00.01

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FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         19514 TO     23446
PROJECTED ANSWERS:              576 TO      1424

L2            50 SEA SSS SAM L1

=>
Uploading C:\Program Files\Stnexp\Queries\PHENYLALANINE INTEGRIN INHs.str
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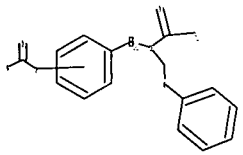

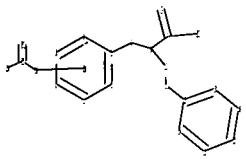

```
chain nodes :
7  8  9  10  11  19  20  24  25  26
ring nodes :
1  2  3  4  5  6  12  13  14  15  16  17
ring/chain nodes :
27
chain bonds :
5-7  7-8  8-9  8-10  9-19  9-20  10-11  11-12  24-25  25-26  25-27
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-13  12-17  13-14  14-15  15-16  16-17
exact/norm bonds :
9-19  9-20  10-11  11-12  24-25  25-26  25-27
exact bonds :
5-7  7-8  8-9  8-10
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-13  12-17  13-14  14-15  15-16  16-17
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
 11:CLASS  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  19:CLASS  20:CLASS
 24:CLASS  25:CLASS  26:CLASS  27:CLASS  28:Atom


L3      STRUCTURE UPLOADED

=> D L3
L3 HAS NO ANSWERS
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```
L3              STR
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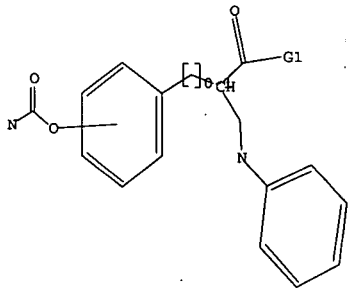


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G1 O,N


Structure attributes must be viewed using STN Express query preparation.


=> S L3 SSS FULL
FULL SEARCH INITIATED 09:01:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      2600 TO ITERATE

100.0% PROCESSED      2600 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L4            0 SEA SSS FUL L3

=> LOGOFF
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:Y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                ENTRY     SESSION
FULL ESTIMATED COST                             167.82     168.03

STN INTERNATIONAL LOGOFF AT 09:01:42 ON 28 DEC 2006
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